UT-BATTELLE

Advanced Neutronics Simulation Development and Directions

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Workshop on High End Computing For Nuclear Fission Science and Engineering

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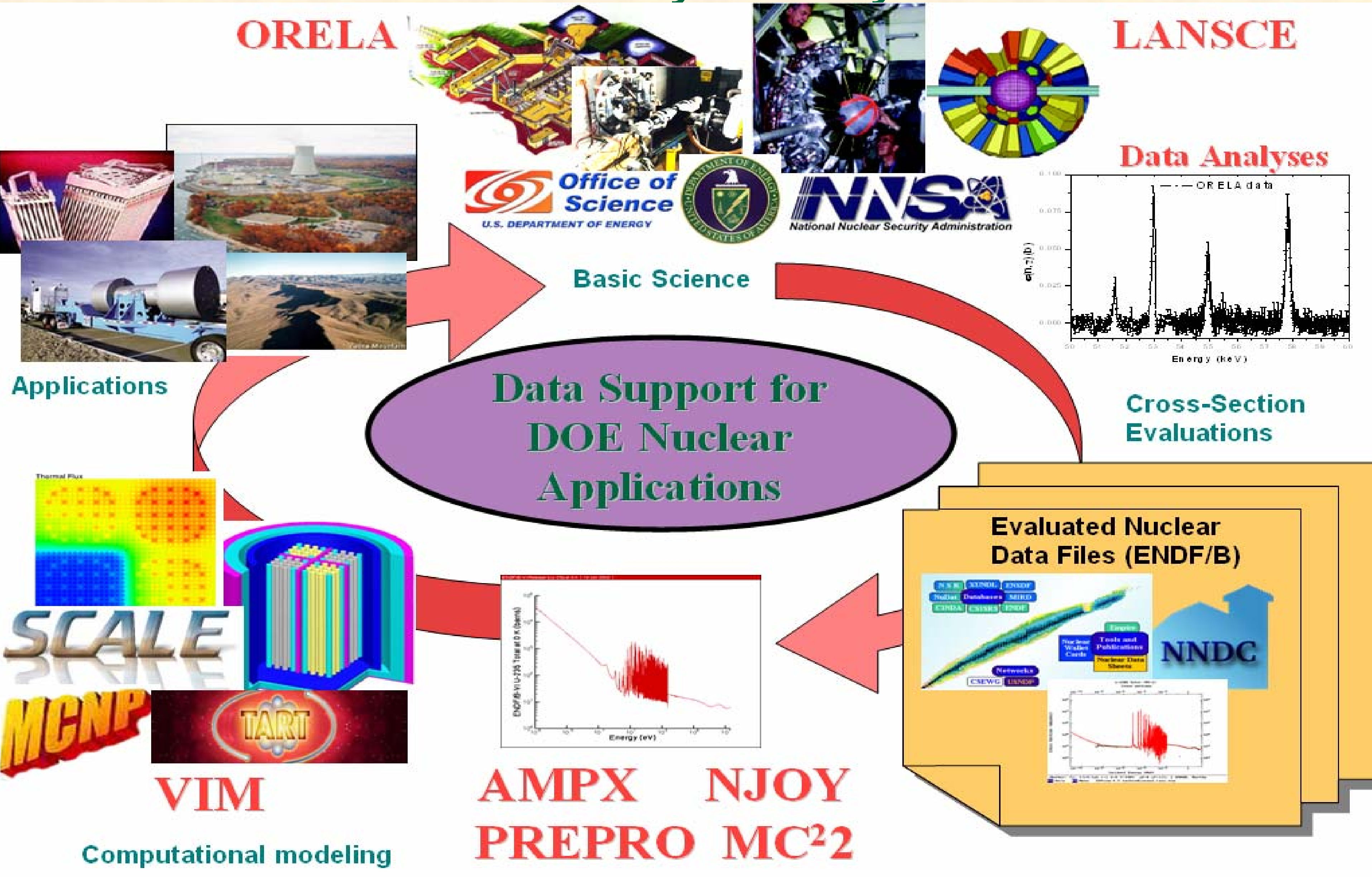
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

NEEDS

- Improved-fidelity/resolution methods
  - Experiments are expensive and facilities are limited or not available. We can't rely on experiments as much as we did in the past.
  - Ranges of applicability are broad, so methods need to be robust and dependable.
- Materials & Fuels are generally the most limiting area for determining design options.
- Supplement/extrapolate experimental data (cross sections, desktop experiments, separate effects rather than system level).
- Validation and assessments of uncertainties and biases are key for licensing and economical operation.
- Reduction in designer effort through automated design methodologies

Infrastructure/Analysis Cycle:



Specfic Examples

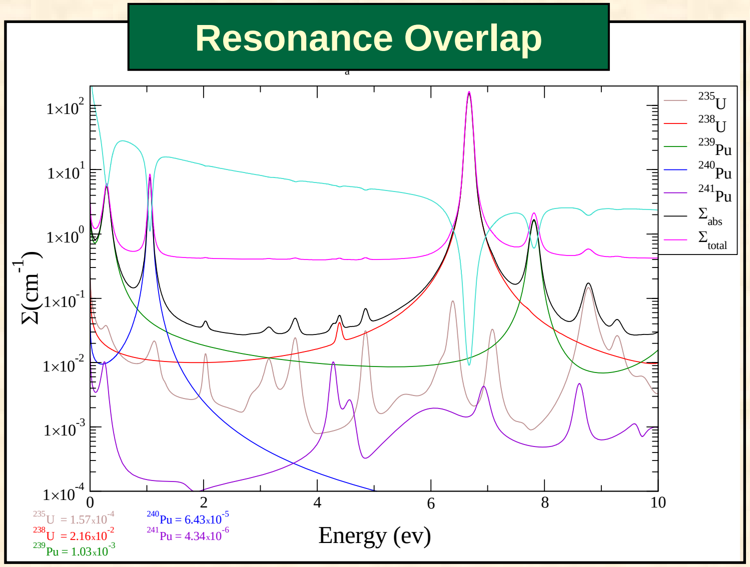
- **Nuclear Data**
- **Energy Treatment**
- **S/U Methods**
- **Optimization**
- **Coupled Physics**

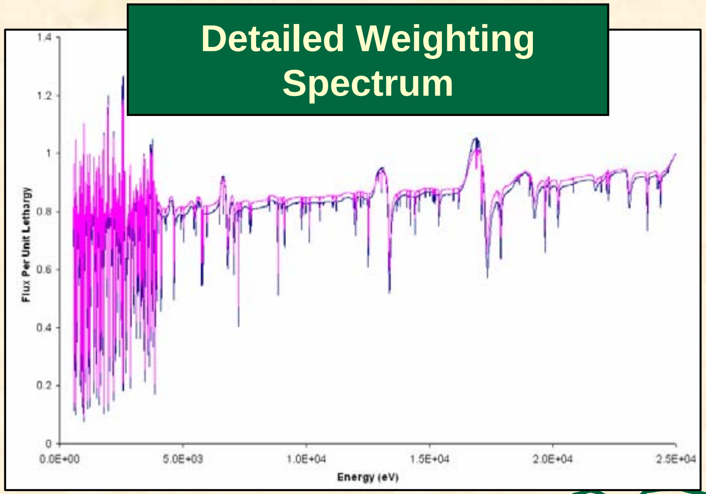
Development and Validation of Temperature Dependent Thermal Neutron Scattering Laws (NERI Project 01-140)

- **Collaborative Project with NCSU (Ayman Hawari)**
- **Update models and models' parameters by introducing new developments in thermalization theory and condensed matter physics**
  - **Use atomistic simulations to compute phonon distribution.**
  - **Use photon distribution in GASKET/LEAPR to compute updated scattering kernels (C, Be, BeO, ZrH, ThH, $(CH_2)_n$, H_2O**
- **Apply updated thermal scattering libraries to benchmark models to determine improvement.**
- **In the case of graphite, perform a benchmark experiment by observing neutron slowing down as a function of temperatures equal to or greater than room temperature**
- **Understand the implications of the obtained results on the ability to accurately determine the operating and safety Characteristics of a given reactor design**

Improved Energy treatment in deterministic codes

- **1-D CENTRM Code introduced in SCALE 5.0**
  - Continuous energy, point-wise library (~30,000 Energy Points)
  - Solve transport equation using Discrete Ordinates Method
  - Solve detailed slowing down problem to obtain multi-group cross sections for Monte Carlo/Lattice Physics Codes

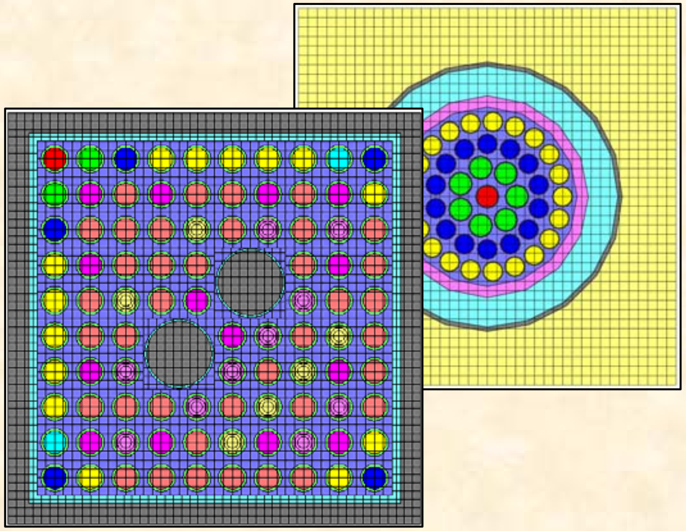


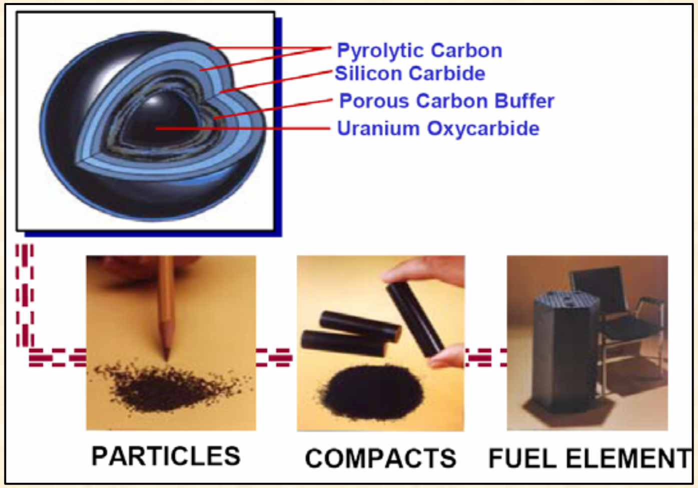


Detailed Energy Treatment – 2-D

- **1-D approximation cannot easily capture non-infinite lattices.**
- **GEMINEWTRN**
  - **Combine 2-D NEWT Extended Step Characteristics method with CENTRM Energy Detail**
  - **Idea for benchmarking more approximate methods**
- **Joint project with Purdue Univ.**

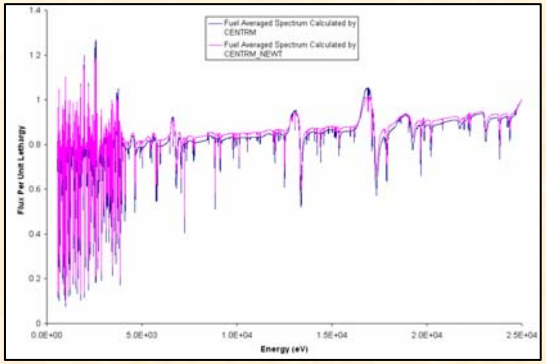
Heterogeneous Designs





TRITON Combines Rigorous Methods

- **CENTRM: 1-D continuous energy resonance processing**
- **ORIGEN-S: detailed isotopic compositions**
- **NEWT: 2-D flexible mesh geometry discrete ordinates transport**
- **Implemented in modular SCALE system**



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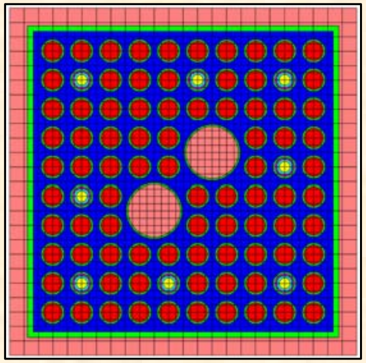

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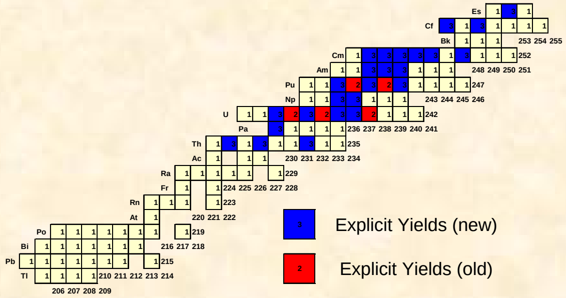


CENTRM (Energy Detail)

NEWT (Spatial/Angular Detail)

ORIGEN-S (Isotopic Detail, 1600 nuclides)

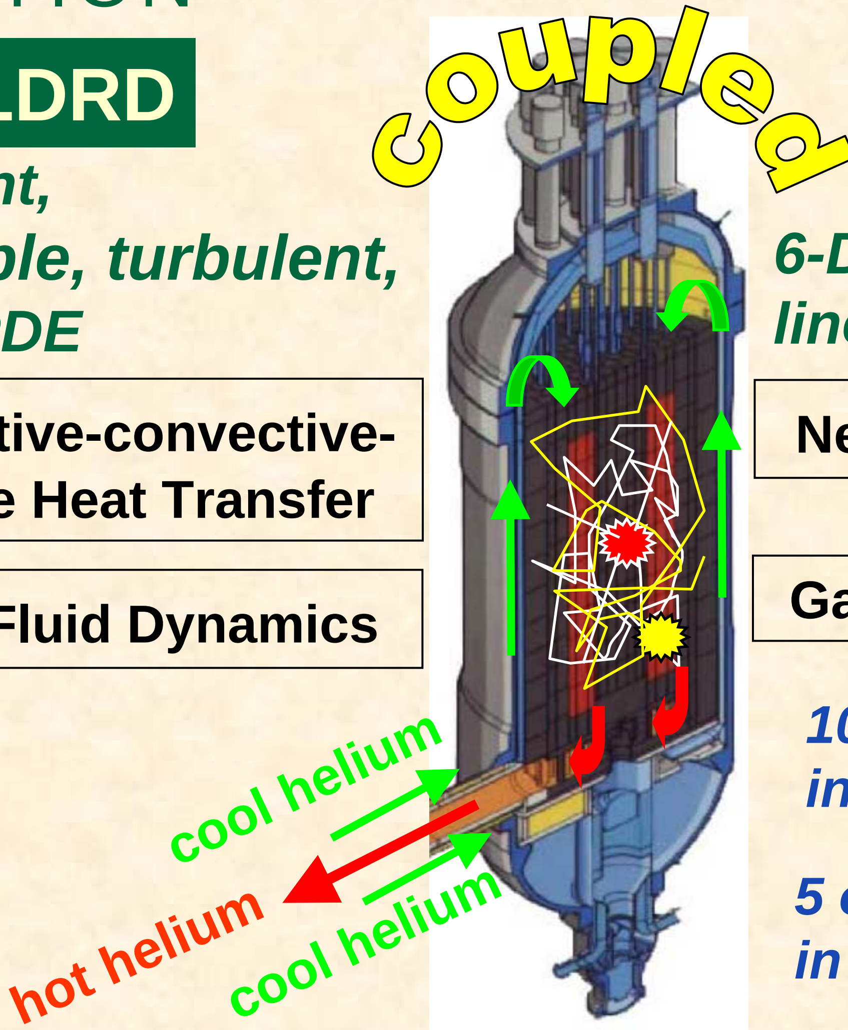
JOINT INL/ORNL LDRDs: FULLY-COUPLED NUCLEAR REACTOR SIMULATION

INL LDRD

3-D, transient, compressible, turbulent, non-linear PDE

Conductive-convective-radiative Heat Transfer

Fluid Dynamics



ORNL LDRD

6-D, transient linear integral-PDE

Neutron Transport

Gamma Transport

10 orders of magnitude in energy

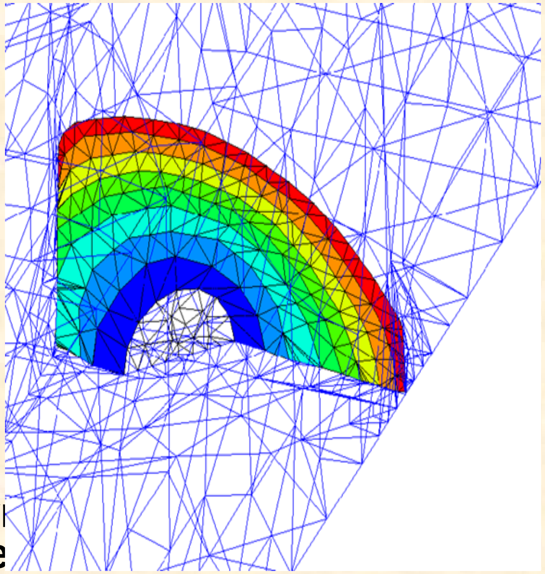
5 orders of magnitude in space

The ORNL LDRD: A HIGH-FIDELITY SIMULATION PACKAGE

- **Develop a high-fidelity radiation transport solver**
  - **Specifically designed for terascale computing**
  - **High-fidelity in both space and energy (based on centrm approach)**
- **Create the computer science infrastructure**
  - **For code efficiency & interoperability in terascale machines**
  - **Leverage existing software:**
    - **DOE's SciDAC software**
    - **ORNL's SCALE nuclear analysis code system**
  - **Teaming with ORNL computer science expertise**
- **Demonstrate the capability**
  - **Develop two visual demonstrations of the software**
    - **Independent radiation transport simulation**
    - **Coupled-physics simulation of a transient**

All built on a comprehensive COMPUTER SCIENCE INFRASTRUCTURE

- **Develop the setup geometry and meshing tools**
  - **Efficient parametric geometric modeling and processing tools**
  - **Advanced terascale grid generation and improvement techniques**
  - **Adaptive parallel hybrid mesh generation**
    - **Flexible mix of structured and unstructured mesh**
    - **AMR within the unified computational basis**
- **Leverage existing SciDAC technology**
  - **Common component architecture**
    - **Extensibility of each physics module**
    - **Interoperability of modules across platforms**
  - **Meshing tools and techniques from TSTT**
- **Domain decomposition and mesh ordering**
  - **Optimized ordering to take advantage of the *a priori* know computational wave fronts in the radiation transport solve**



Validation, Experiments, and S/U

- **Good experiment data for code validation is hard to find for advanced reactor systems, a couple of key activities:**
  - **International Criticality Safety Benchmark Evaluation Project**
  - **International Reactor Physics Benchmark Experiments**
- **S/U tools can be used to determine:**
  - **What is important, which cross sections to measure**
  - **Fundamental assessment of uncertainties from basic data to support margins**
  - **Determine the applicability of experiments**
  - **Can be used to perform cross section adjustments to improve accuracy**
  - **Calculation of uncertainties requires significantly more computing time that the calculation of the value of interest.**

Optimization for Design

- **Current example is fuel loading**
- **With multi-physics, multi-component can apply optimization methods for automated design**
  - **Eliminate current iteration performed between particular areas of expertise**
  - **Computing intensive: requires multiple calculations**
  - **Optimize on economics, reliability, proliferation resistance**
- **Some general-purpose tools already exist (e.g. DAKOTA)**

Nuclear Technology End station Concept

1. **Approach for National Leadership Computing Facility - Complete simulation tool set on a HPC**
2. **Concept for reactor design and analysis:**

RADIATION TRANSPORT

Neutron
Photon

CONTINUUM MECHANICS

Multi-phase CFD
Heat transfer
Chemically reactive flow
Fluid-structure dynamics

3. **Add components for broader NS&T community**

RADIATION TRANSPORT

Charged-Particle
Spallation Physics

CONTINUUM MECHANICS

Elasto-plastic dynamics
Impact dynamics
Radiation damage in materials